Phenomenological lattice model for dynamic spin and charge fluctuations in the cuprates

Matthias Vojta
Institut für Theorie der Kondensierten Materie, Universität Karlsruhe, 76128 Karlsruhe, Germany.

Subir Sachdev
Department of Physics, Yale University, P.O. Box 208120, New Haven CT 06520-8120, USA.

(Dated: August 20, 2004)

Motivated by recent neutron scattering experiments on the cuprate superconductors, we present a phenomenological framework describing the dynamics of collective spin excitations coupled to charge/bond order fluctuations. Our quantum lattice model contains two order parameter fields, and can capture spin excitations both in broken-symmetry states with static lattice modulations, as well as in homogeneous states where the charge/bond order is fluctuating. We present results for different types of static charge/bond order, namely site- and bond-centered stripes, and plaquette modulation.

I. INTRODUCTION

For certain cuprate high-temperature superconductors it has been established that incommensurate spin and charge correlations, commonly referred to as stripes, appear over a significant range of the phase diagram[1,2,3]. The role of these stripes both for superconductivity itself as well as for various anomalies in the normal state has been discussed extensively[4,5,6,7,8,9,10], but is at present not fully understood.

Recent neutron scattering experiments[11,12,13,14] have mapped out spin excitations in various cuprates over a large range of energies. Tranquada *et al.*[11] investigated the excitation branches in $La_{2-x}Ba_xCuO_4$ at a hole doping of $x = \frac{1}{8}$, which displays static spin and charge order, up to energies of 200 meV. They found the high-energy part to be well described by the spectrum of spin ladders, pointing towards bond order in the material[15,16]. Remarkably, other cuprate families like $YBa_2Cu_3O_{6+y}$ or $Bi_2Sr_2CaCu_2O_{8+\delta}$, where charge order remains dynamically fluctuating, show a very similar spin excitation spectrum at elevated energies. (At low energies, the spectrum depends on whether the system shows static order; furthermore, the strength of electronic quasiparticle damping is different between different compounds, limiting the wavevector range where sharp single-particle excitations can be seen.) These experiments raise the question of whether there exists a dynamic spin response which is *universal* among all cuprates: namely a high-intensity ("resonance") peak at wavevector (π, π) and energy between 20 and 50 meV, with both downward and upward dispersing branches of excitations.

The purpose of this paper is to develop a unified theoretical framework for describing spin excitations in the presence of both static and dynamic charge order. We will do this using a phenomenological lattice model. Our approach differs from previous phenomenological theories[17,18,19] in two important ways: (*i*) These theories took the continuum limit for spin modulations in the vicinity of the incommensurate spin-ordering wavevector; such a theory is not expected to be valid near the resonance peak at (π, π). We will instead use a lattice model which is valid both at (π, π) and near the incommensurate wavevector, and for a wide range of energies. (*ii*) Our model explicitly selects *collinear* spin correlations, in contrast to the previous approaches[17,19] where the distinction between collinear and spiral spin correlations only appears in higher order terms which are not fully accounted for in existing calculations.

Our model is an extension of recent microscopic spin-only models for stripe phases[15,16] which have quite successfully modelled some of the neutron scattering data.[11] One of our purposes is to judge the significance of this agreement between theory and experiment: in particular, we wish to delineate the range of models which are compatible with the data, including those which cannot be described by simple spin-only Hamiltonians. Furthermore, our approach can be naturally extended to the case where the charge order is dynamic, rather than the static order needed to define the models of Refs. 15,16.

We will model spin and charge fluctuations on a phenomenological basis using Landau order parameters for both. The coupling between the two orders can shift the minimum energy of the spin excitations from (π, π) to the incommensurate wavevector dictated by the charge order. On a microscopic scale, the influence of the charge order on the spin sector can be understood in terms of both spatially modulated spin densities and spatially modulated couplings, as found in the models of Refs. 15,16. Our Landau-like theory will be formulated directly on the underlying square lattice, which will allow us to capture lattice effects such as the differences between site-centered or bond-centered order. Importantly, the spin sector described by our theory will be strongly fluctuating, *i.e.*, we are far from the semiclassical limit described by spin waves[18,20,21]. Microscopically, these fluctuations can arise from the tendency to dimerization, *i.e.*, from *bond order*, which is present in the undoped paramagnetic parent Mott insulator[9,22]. (Note that bond order can occur both in site-centered and bond-centered stripe states.)

II. QUANTUM LATTICE MODEL

We assume a dominant antiferromagnetic interaction between the spins, and so model the quantum spin fluctuations by a standard vector φ^4 Landau theory for the antiferromagnetic order parameter at the *commensurate* wavevector $\mathbf{Q} = (\pi, \pi)$. So on a square lattice of sites, j, we parameterize the lattice spins by

$$S_{j\alpha} \propto e^{i\mathbf{Q}\cdot\mathbf{r}_j}\varphi_{j\alpha} \tag{1}$$

where $\alpha = x, y, z$. In the absence of any coupling to charge/bond order, we assume that the dominant spin fluctuations remain at the commensurate $\mathbf{Q}$; we find below that this feature is important in obtaining a resonance peak at $\mathbf{Q}$. The effective action for these commensurate spin fluctuations has a familiar form:

$$\begin{aligned}\mathcal{S}_0 &= \int d\tau \sum_j \left[\frac{1}{2}\left(\frac{\partial\varphi_{j\alpha}}{\partial\tau}\right)^2 + \frac{s}{2}\varphi_{j\alpha}^2 + \frac{u}{4}\left(\varphi_{j\alpha}^2\right)^2\right] \\ &+ \int d\tau \sum_{\langle jj'\rangle} \frac{c^2}{2}\left(\varphi_{j\alpha} - \varphi_{j'\alpha}\right)^2 \end{aligned} \tag{2}$$

In principle, there should also be Berry phases in the quantum spin action, but we assume that they have averaged out to zero: this is expected to be valid in the compressible superconducting states, or in the incompressible Mott insulators with an even number of electrons per unit cell, but likely not at the quantum critical point between such phases.

Now we include the effect of charge/bond order. This we represent by the complex continuum fields $\phi_{x,y}(\mathbf{r}, \tau)$ which measure the amplitude of charge order at the wavevectors $\mathbf{K}_x = (\pi/2, 0)$ and $\mathbf{K}_y = (0, \pi/2)$ – this is the dominant ordering wavevector of the Mott insulating state at 1/8 doping, and is therefore the appropriate reference wavevector for our considerations: we will show below how deviations in the charging ordering wavevector from $\mathbf{K}_{x,y}$ in the superconducting phases (or at non-zero temperatures) can be easily built into our formalism. Using the complex order parameters $\phi_{x,y}$, it is convenient to define the real field

$$Q_x(\mathbf{r}) = \phi_x(\mathbf{r})e^{i\mathbf{K}_x\cdot\mathbf{r}} + \phi_x^*(\mathbf{r})e^{-i\mathbf{K}_x\cdot\mathbf{r}} \tag{3}$$

and similarly for Q_y. For $\mathbf{r}$ on the sites of the square lattice, the $Q_{x,y}$ are measures of the charge density modulation on those sites. On the other hand, for $\mathbf{r}$ on the links of the square lattice, the $Q_{x,y}$ is a measure of the local *bond* order: this is determined by the modulation in the local pairing amplitude or exchange energy. With these physical interpretations at hand, we can write down the following couplings between the spin and charge fluctuations

$$\begin{aligned}\mathcal{S}_x = \int d\tau \sum_j \Big[&\lambda_1 Q_x(\mathbf{r}_j)\varphi_{j\alpha}^2 + \lambda_2 Q_x(\mathbf{r}_{j+x/2})\varphi_{j\alpha}\varphi_{j+x,\alpha} \\ &+\lambda_3 Q_x(\mathbf{r}_j)\varphi_{j-x,\alpha}\varphi_{j+x,\alpha} + \lambda_4 Q_x(\mathbf{r}_{j+y/2})\varphi_{j\alpha}\varphi_{j+y,\alpha}\Big]\end{aligned} \tag{4}$$

with four independent couplings constants λ_{1-4}; the same couplings will appear in the corresponding $\mathcal{S}_y$. Notice that λ_1 implements the correlation between the onsite charge density and the amplitude of the spin fluctuations, while λ_{2-4} ensure that the effective first- and second-neighbor exchange constants controlling the spin correlations modulate along with the bond order.

If we now take $\phi_{x,y}$= constant, then the action $\mathcal{S}_0$+$\mathcal{S}_{x,y}$ represents our general theory for quantum spin fluctuations in a background of static charge/bond order. The site-centered case has $\phi_x = 1$, and the bond-centered case has $\phi_x = e^{i\pi/4}$. Two-dimensional (plaquette or checkerboard) order will have both ϕ_x and ϕ_y non-zero. At the Gaussian level ($u = 0$), the problem is quadratic in the φ fields, and can be solved by diagonalizing a matrix of size $(N_xN_y)^2$, where $N_{x,y}$ describe the size of the unit cell (in the charge sector).

For large enough λ couplings, the minimum energy of the φ fluctuations will be shifted away from (π, π), as observed in experiment. Notably, the restriction to *real* φ implies that the spin order remains collinear. For small mass s, the spin order can condense as usual, and fluctuations around the condensate will lead to low-energy Goldstone modes.

A. Fluctuating charge order

The above formalism is designed to allow easy extension to the dynamic charge order case, which is likely relevant for $YBa_2Cu_3O_{6+y}$ and $Bi_2Sr_2CaCu_2O_{8+\delta}$. We use a continuum formulation to describe the charge fluctuations, with the following general action consistent with all the symmetries of the lattice:

$$\begin{aligned}\mathcal{S}_\phi = \int d\tau d^2\mathbf{r}\Big[&|\partial_\tau\phi_x|^2 + |\partial_\tau\phi_y|^2 + c_1^2|\partial_x\phi_x|^2 \\ &+c_2^2|\partial_y\phi_x|^2 + c_1^2|\partial_y\phi_y|^2 + c_2^2|\partial_x\phi_y|^2 + i\delta\phi_x^*\partial_x\phi_x \\ &+i\delta\phi_y^*\partial_y\phi_y + s_1\left(|\phi_x|^2 + |\phi_y|^2\right) + u_1\left(|\phi_x|^4 + |\phi_y|^4\right) \\ &+v|\phi_x|^2|\phi_y|^2 + w\left(\phi_x^4 + \phi_x^{*4} + \phi_y^4 + \phi_y^{*4}\right)\Big]\end{aligned} \tag{5}$$

Note especially the term proportional to δ: it is generically present, and when the strength of the charge order is weak it ensures that the dominant charge order fluctuations are at an incommensurate wavevector unequal to $\mathbf{K}_{x,y}$. However at low temperatures (T) in an insulating state, the 'lock-in' term proportional to w eventually dominates, and selects a commensurate charge-ordered state with wavevectors equal to $\mathbf{K}_{x,y}$. The quartic v term determines whether the long-range order will be one-dimensional ("stripe") or two-dimensional ("plaquette", "checkerboard").

The effect of charge fluctuations on the spin excitation spectrum can now be determined by self-consistently computing the frequency and momentum dependence of the φ_α self energy to second order in the λ's, similar to Ref. 23. A full calculation along this line is beyond the

scope of this paper, we expect that in the limit of small mass s_1 the results will be similar to the ones obtained in the static ϕ theory.

B. Coupling to phase fluctuations

An advantage of the present phenomenological formalism is that is allows easy extension to include couplings to other collective modes. If the cuprate compound is a superconductor, then there is an additional mode associate the fluctuation of θ, the phase of the superconducting order. As in Ref. 24, the most relevant coupling of θ to the spin fluctuations is

$$\mathcal{S}_{\varphi\theta} = \int d^2r d\tau \left[i\gamma \partial_\tau \theta \varphi_\alpha^2 \right] \tag{6}$$

The action for θ fluctuations can be generally written as[25]

$$\mathcal{S}_\theta = \int \frac{d^2k d\omega}{8\pi^3} (K_1 k^\sigma \omega^2 + K_2 k^2) |\theta(k,\omega)|^2 \tag{7}$$

where k is a wavevector and ω is an imaginary frequency, and the parameter σ is determined by the nature of the Coulomb interaction: for screened short-range interactions $\sigma = 0$, while for in-plane $1/r$ Coulomb interactions with independent layers $\sigma = 1$. In a paramagnetic state where φ_α excitation forms a sharp $S = 1$ 'triplon' excitation, the coupling to phase fluctuations will induce damping in the triplon spectral function. At $T = 0$, and at the bottom of the triplon band, it is not difficult to compute from Eqs. (6,7) that the imaginary part of the triplon self energy is $\sim (\epsilon - \Delta)^{2(d-\sigma)/(2-\sigma)}$ at the bottom of the band ($\epsilon \geq \Delta$ is real frequency and Δ is the spin gap): this arises from the 'radiation' of θ excitations by the triplon.

III. RESULTS FOR STATIC CHARGE ORDER

Let us now present a few result for the case of static charge/bond order, calculated in the Gaussian approximation of $\mathcal{S}_0 + \mathcal{S}_x + \mathcal{S}_y$. We directly calculate the $T = 0$ susceptibility as measured in inelastic neutron scattering. In the following, we restrict our attention to the one-particle contributions, as the multiparticle continuum will be hard to detect experimentally. Averaging over the neutron spin polarizations, we obtain the dynamic spin susceptibility $\chi''(\mathbf{k}, \omega)$ as sum of δ peaks with weights determined by various matrix element terms.

In order to compare with the experiment of Ref. 11 we add the contributions from horizontal and vertical charge modulations (Figs. 1 and 2), and plot the result as function of the external momentum at fixed energy, furthermore we broaden the δ peaks to account for the experimental resolution.

In Figs. 1 and 2 we show the response for bond- and site-centered stripe structures, where the parameters are

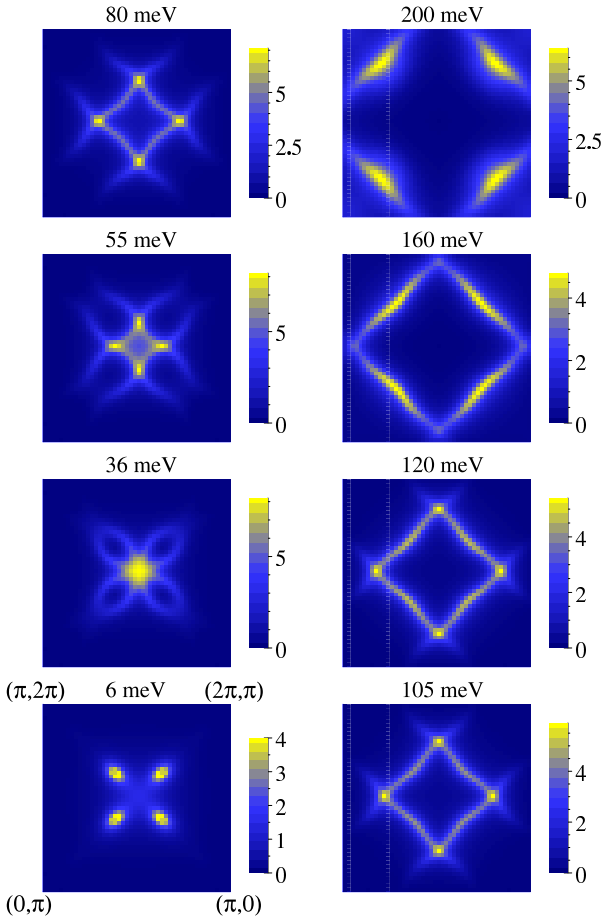

FIG. 1: (color) Neutron scattering intensity, $\chi''(\mathbf{k}, \omega)$, for a state with bond-centered charge order. Parameter values are $c = 160$ meV, $\lambda_1|\phi_x| = 100$ meV, $\lambda_2|\phi_x| = 600$ meV, $\lambda_3 = \lambda_4 = 0$. $s = 550$ meV is choosen is place the spin sector at its critical point. The panels show fixed energy cuts as function of momentum in the *magnetic* Brillouin zone. The δ peaks have been replaced by Lorentzians with width $\Gamma = 15meV$, and the responses of horizontal and vertical stripes have been added. The figure can be directly compared to Fig. 2 of Ref. 11.

chosen to match the experimental result of Ref. 11. The coupling between charge and spin sector is captured by λ_1 which modulates the spin density, and in $\lambda_{2,3}$ which induce a spatial variation in the exchange couplings. As in Refs. 15,16, we observe a "dual" character of the lowest spin excitation branch: For small energies (*e.g.* 6 meV) the response consists of four peaks representing the four cones of spin-wave modes. With increasing energy the cones widen; however, the outer part becomes suppressed in intensity due to matrix element effects. Around 30 – 50 meV the spectrum is dominated by the strong response near (π, π) ("resonance peak"), which arises from a saddle point of the mode dispersion. For higher energies, the modes gradually change their character towards a one-dimensional excitation spectrum, and the scattering intensity forms a diamond which moves outward with in-

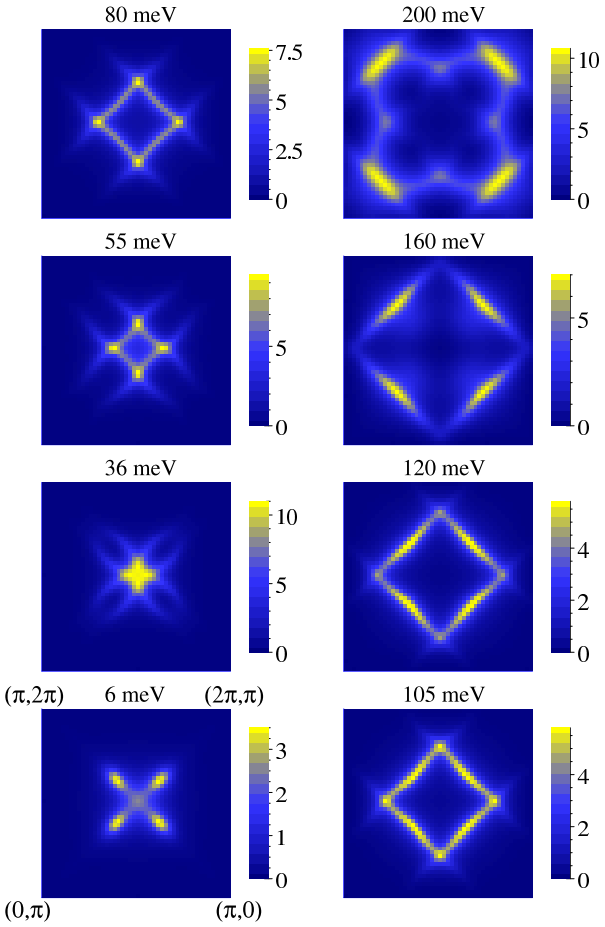

FIG. 2: (color) As Fig. 1, but now for a state with *site*-centered charge order, and parameter values are $\lambda_1|\phi_x| = 200$ meV, $\lambda_3|\phi_x| = 100$ meV, $\lambda_2 = \lambda_4 = 0$, and $s = 140$ meV. Again the responses of horizontally and vertically ordered states have been added.

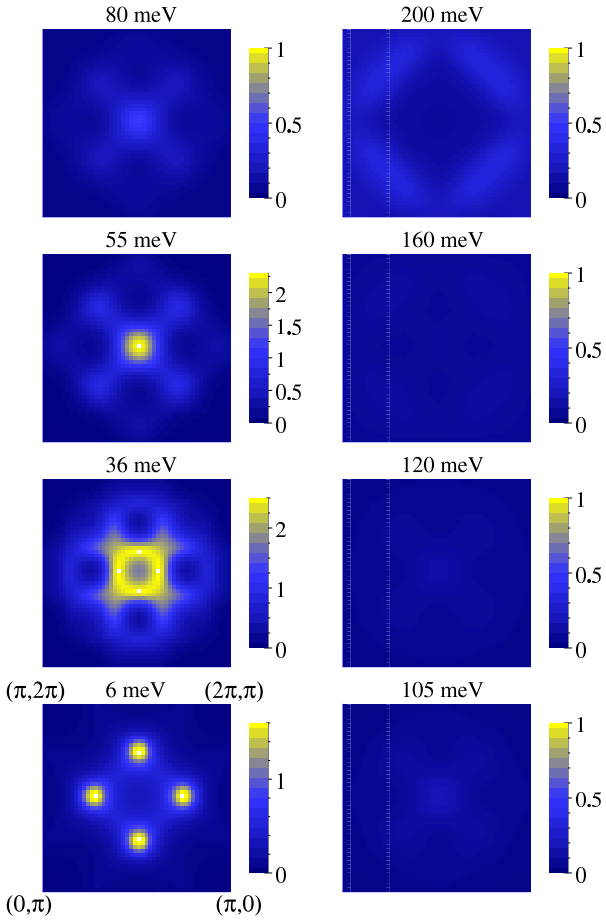

FIG. 3: (color) As Fig. 1, here for a state with two-dimensional *plaquette* charge order. Parameters are $\lambda_1|\phi_x| = 100$ meV, $\lambda_2|\phi_x| = 600$ meV, $\lambda_3 = \lambda_4 = 0$, and $s = 1.3$ eV. The spin order condenses at wavevectors $(\pi \pm \pi/4, \pi \pm \pi/4)$ instead of $(\pi \pm \pi/4, \pi)$, $(\pi, \pi \pm \pi/4)$. Furthermore the dispersion features a single energy scale only, i.e., there is no magnetic response above the saddle point at (π, π). (A higher band of spin excitations start around 250 meV.)

creasing energy. Overall, there is reasonable agreement with the experimental data of Tranquada *et al.*[11]. A crucial point is the presence of two energy scales in the dispersion: a bandwidth of about 250 meV arising from the strong coupling along the stripes, and a saddle point at about 40 meV whose energy is dictated by the coupling across the stripes and the deviation of the ordering wavevector from (π, π). Remarkably, the difference between the bond- and site-centered situation are minimal, i.e., the is little distinction on symmetry grounds. (Microscopically, however, strong spin fluctuations which drive the system away from the quasiclassical limit are favored in a bond-centered geometry[15,16,26,27].)

Fig. 3 shows the result for bond-centered checkerboard order, with microscopic parameters similar to Fig. 1. Clearly, the result is completely different: The low-enery modes appear at four points rotated by 45 degrees compared to Figs. 1, 2, and the dispersion shows only a single energy scale. Thus, the "dual" character of the spectrum is absent here.

IV. CONCLUSIONS

We have presented a general quantum lattice model which describes spin excitations in the presence of either static or fluctuating charge/bond order.

In the case of anisotropic ('one-dimensional') charge order, the magnetic modes resemble semi-classical spin waves at low energies, but cross over into triplon excitations of a quasi-one-dimensional quantum paramagnet at higher energies. The crossover energy, associated with a saddle point in the mode dispersion, is only a fraction of the bandwidth for systems close to a magnetic quantum phase transition. Two ingredients are crucial for the "dual" character of the modes: (*i*) strong quantum fluctuations, and (*ii*) the presence of two energy scales in the dispersion. We found that the spectrum was relatively insensitive to the bond- or site-centered nature of the charge order. We also examined fully two-dimensional

'plaquette' ordered states, and found that they could not describe the experimental observations.

An interesting open question is the precise link between the neutron scattering observations and the modulations observed in recent STM experiments.[28,29,30,31] In principle, our approach can be adapted to any specific charge order observed in STM, and can then compute its spin excitation spectrum. It is already clear from our results that at least in $La_{2-x}Ba_xCuO_4$, the charge order cannot be strictly a two-dimensional 'checkerboard' structure: anisotropic "quasi-one-dimensional" correlations over some finite range appear to be required.

Acknowledgments

We thank S. Kivelson, A. Polkovnikov, S. Scheidl, J. Tranquada, G. Uhrig, and T. Ulbricht for illuminating discussions and collaborations on related work. This research was supported by the National Science Foundation under grants DMR-0098226 (S.S.) and DMR-0210790, PHY-9907949 at the Kavli Institute for Theoretical Physics (M.V., S.S.) and the DFG Center for Functional Nanostructures Karlsruhe (M.V.).

[1] J. M. Tranquada *et al.*, Phys. Rev. Lett. **78**, 338 (1997); J. M. Tranquada, J. Phys. Chem. Solids **59**, 2150 (1998).
[2] P. Dai *et al.*, Phys. Rev. Lett. **80**, 1738 (1998); H. A. Mook *et al.*, Phys. Rev. Lett. **88**, 097004 (2002).
[3] S. Wakimoto *et al.*, Phys. Rev. B **64**, 174505 (2001).
[4] V. J. Emery *et al.*, Phys. Rev. B **56**, 6120 (1997).
[5] V. J. Emery, S. A. Kivelson, and J. M. Tranquada, Proc. Natl. Acad. Sci. USA **96**, 8814 (1999).
[6] J. Zaanen, Nature **404**, 714 (2000).
[7] D. J. Scalapino and S. R. White, Foundations of Physics **31**, 27 (2001).
[8] J. Zaanen, J. Phys. Chem. Solids **59**, 1769 (1998); J. Tworzydlo *et al.*, Phys. Rev. B **59**, 115 (1999).
[9] S. Sachdev, Rev. Mod. Phys. **75**, 913 (2003).
[10] S. A. Kivelson *et al.*, Rev. Mod. Phys. **75**, 1201 (2003).
[11] J. M. Tranquada *et al.*, Nature **429**, 534 (2004).
[12] V. Hinkov *et al.*, Nature **430**, 650 (2004).
[13] C. Stock *et al.*, cond-mat/0408071.
[14] S. M Hayden *et al.*, Nature **429**, 531 (2004).
[15] M. Vojta and T. Ulbricht, cond-mat/0402377.
[16] G. S. Uhrig, K. P. Schmidt, and M. Grüninger, cond-mat/0402659.
[17] O. Zachar, S. A. Kivelson, and V. J. Emery, Phys. Rev. B **57**, 1422 (1998).
[18] C. D. Batista, G. Ortiz, and A. V. Balatsky Phys. Rev. B **64**, 172508 (2001).
[19] Y. Zhang, E. Demler and S. Sachdev, Phys. Rev. B **66**, 094501 (2002).
[20] F. Krüger and S. Scheidl, Phys. Rev. B **67**, 134512 (2003)
[21] E. W. Carlson *et al.*, cond-mat/0402231.
[22] S. Sachdev and N. Read, Int. J. Mod. Phys. B **5**, 219 (1991); M. Vojta and S. Sachdev, Phys. Rev. Lett. **83**, 3916 (1999).
[23] A. P. Kampf and J. R. Schrieffer, Phys. Rev. B **42**, 7967 (1990).
[24] E. Frey and L. Balents, Phys. Rev. B **55**, 1050 (1997).
[25] M. P. A. Fisher and G. Grinstein, Phys. Rev. Lett. **60**, 208 (1988).
[26] V. I. Anisimov *et al.*, cond-mat/0402162.
[27] G. Seibold and J. Lorenzana, cond-mat/0406589.
[28] M. Vershinin *et al.*, Science **303**, 1995 (2004).
[29] C. Howald *et al.*, Phys. Rev. B **67**, 014533 (2003).
[30] K. McElroy *et al.*, cond-mat/0404005.
[31] T. Hanaguri *et al.*, unpublished.